#### **EURASIAN JOURNAL OF MATHEMATICAL AND COMPUTER APPLICATIONS** ISSN 2306–6172 Volume 5, Issue 2 (2017) 36–65

#### STUDY OF THE RAYLEIGH-BÉNARD INSTABILITY BY METHODS OF THE THEORY OF NONEQUILIBRIUM PHASE TRANSITIONS IN THE CAHN-HILLARD FORM

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**Abstract** The paper reconstructs the early stage of the Rayleigh–Bénard convective instability considered as a nonequilibrium phase transition with the spinodal decomposition (diffusion separation) mechanism

**Key words:** Rayleigh-Benard instability, nonequilibrium phase transitions, the Kahn-Hillard model, diffusion fibration, the Ginzburg-Landau potential, Gibbs free energy.

AMS Mathematics Subject Classification: 76E09, 76F35, 82C26.

### 1 Introduction

The appearance of convective flows and their evolution from regular forms to eventual transition to irregular ones (the turbulent flows) are of great interest because they are responsible for the efficiency of many engineering heat and mass transfer processes [1], [2]. Such processes are fundamental in chemistry, petrochemistry, energy and metallurgy industries, and in other branches of industry. Convective flows appear in liquids and gas in a gravitational field with spatial inhomogeneity of density created by the inhomogeneity of the temperature and component concentration, which appear, for example, in the course of chemical reactions or due to other causes [3]–[5]. As the difference of temperatures increases, the liquid at rest loses stability, which eventually results in the appearance of convective flows. A further increase in the difference of temperatures leads to the instability of the primary convective flow, while the heat conduction crisis is consequent on the hydrodynamic crisis. The resulting secondary convective flow may also become unstable, a sequence of such crises may result in a turbulent flow [1], [2]. Such problems have been extensively studied (see, in particular, the books [6]–[13]).

The constant interest in problems of such kind, and in particular, in the problem of Rayleigh–Bénard instability is spurred by the significant role they play in new practical applications. For example, in [13], [14] it is noted that beyond the "pure" hydrodynamics formation of space-periodic-type structures is observed during crystal growth, propagation of solidification fronts, electrochemical instabilities of nematic liquid crystals, chemical reaction-diffusive processes, auto-catalytic reactions, bending of thin plates and shells, and in many other problems. Besides, it is assumed that the hydrodynamic approach, which is based on the Boussinesq model, does not apply under low-gravity conditions [15]–[18]. Development of many applications calls for a more subtle theoretical analysis, and in particular, requires finding criteria for distinguishing mechanisms are seen to be in conflict.

the thermo-gravitational Rayleigh–Bénard instability [13], [14] and the thermocapillary Bénard–Marangoni instability [19]. An analysis of experimental data of [1] shows that in a thin layer the vertical differential of temperature is small, and hence, the Rayleigh instability does not develop, whereas the Marangoni instability is realized. In more thick layers, the contribution of the Marangoni instability is small, the instability being developed by the Rayleigh mechanism. On the intermediate thickness scale the

The interest in the problems of joint motion and stability of two or more liquid media with contact along some surface comes from their use in engineering applications. The appearance and character of convective flows in such systems depend on various factors. Either the free-convection or the thermocapillary mechanism can be prevailing depending on the size of the system and the relation between the parameters of the media in contact (see [1], [20], [21] and the bibliography cited therein). Under constant gravity conditions, the thermocapillary motion is as a rule suppressed by the gravitational convection. However, the Marangoni effect plays an important role in cases of microflows of liquid. Under low gravity conditions (at a space station), the thermocapillary convection is one of the principal forms of liquid motion. In solving applied problems, it is important to known which of the convection excitation mechanisms is predominant and what is its effect on the characteristics of the convective flows that appear under the joint action of the gravitation and Marangoni forces. In this case, the effect of such factors as the magnetic field, vibrations, rotations, involved geometry of a system, etc., is increasing.

At the same time, practical applications call for the solution of more and more involved "classical" problems. For example, of special interest for the dynamics of seasonal circulation in reservoirs is the Rayleigh–Bénard problem with anomalous dependence of the water density on temperature [22]. Development of nanotechnologies calls for the consideration of the behavior of thin films, when a heating from below results in their disruption and formation of interlacing "dry" and "nondry" regions or droplets connected by ultrathin films [23]–[26]. Besides, there a number of problems in which this type of the instability problem of a liquid layer is incorporated in a more general heat-mass transfer problem—for example, for evaporation of a light fraction from a multi-component mixture, resulting in a variation of the temperature and an increasing concentration near the surface [5], [27]. The problem of current-stability of a binary electrolyte between two horizontal ion-selective membranes [28] can also be subsumed under the class of such problems with more involved setting.

The complication of practical problems, which may involve, as a single block, problems of liquid instability and convection onset, on one side, and the development of methods of simulation and numerical experiments with high performance numerical methods and fast computers, on the other side, calls for the creation of a generalized approach to simulation and interpretation of the results of numerical and full-scale experiments. Attempts to design such a generalized approach were made earlier, for example, by considering a great number of cooperative phenomena with instability as phase transitions [29]. In turn, phase transitions in various systems can be treated from unified thermodynamic positions (thermodynamics of nonequilibrium phase transitions) [30]–[32]. The approach developed in [30]–[32] depends on the assumption that any system can be characterized both in the stable or in the unstable states by the thermodynamic Ginzburg–Landau potential, which has the form of a free Gibbs–Helmholtz energy. In the present paper, our task is to extend this approach to the Rayleigh–Bénard problem. In this setting, the system consisting of a liquid layer heated from below is first considered as a thermodynamically unstable, having the excessive (potential) energy in the field of gravity, which can be transformed into the hydrodynamic component of the convective flow. It is worth noting that the Rayleigh–Bénard problem was posed in this "thermodynamic" way in [31]. However, the approach of [30]–[32] has principal differences from the "entropy" approach of [31], because the free energy is used as a principal characteristic of the behavior of the system (the entropy enters as a term in the Gibbs–Helmholtz equation and is a new, but not unique, thermodynamic quantity, which controls the behavior and dynamics of the system). Besides, the approach of [28]–[30] depends on the thermodynamic formalism of the theory of Cahn–Hillard nonequilibrium processes [34]–[43], which was later developed in [44], [45].

The Rayleigh–Bénard problem is stated as follows. Assume that there is a horizontal layer of liquid of infinite length [29]. The temperature gradient is maintained by underneath heating. When expressed in appropriate dimensionless units, this gradient is called the Rayleigh number Ra. For relatively small Rayleigh number the liquid is calm and the heat is transported by conductance. However, if Ra exceeds some threshold, then a convective flow suddenly develops in the liquid. Convective structures are known to be quite regular and may form either cylindrical or hexagonal configurations. (The top view of a convective cell is a hexagon.) The liquids rises in the cell center and descends near its boundaries, or vice versa. The problem is to explain the mechanism of this sudden "disorder–order" transition and to predict the form and stability of cells.

A more fine theory requires the consideration of fluctuations. The problem is closely related with Taylor vortexes, which appear in the liquid layer between an extended fixed cylinder and a rotating concentric inner cylinder. If the rotation rate of the inner cylinder, as expressed in appropriate dimensionless units (the Taylor number), is sufficiently small, then the liquid flows along streamlines (the Couette flow). However, if the Taylor number exceeds certain critical value, then periodic (Taylor) vortexes will appear along the axial direction.

The principal physical quantities in this problem (the Bénard cells) is the field of velocities at a point (x, y, z), the pressure p, and the temperature T. The field of velocities, pressure and temperature obey certain nonlinear hydrodynamic equations, which can be reduced to a form that explicitly depends on the Rayleigh number Ra (which is an external parameter). For small values of Ra the solution is obtained on assuming that the velocity components are zeros. The stability of this solution is verified by linearization of all equations with respect to the stationary values of the velocities, pressure, temperature—in this way arrive at decaying waves. However, the solutions become unstable if the Rayleigh number exceeds a certain threshold  $Ra_{cr}$ . The unstable solutions define a set of modes. The real field of velocities and temperatures can be expanded into these modes with unknown amplitudes. An important thing here is that for mode amplitudes we get nonlinear equations generating certain configurations created by stable modes. Considering thermal fluctuations, we arrive at the problem

involving deterministic and fluctuating forces. It is worth pointing out that their joint action defines the transition region, where  $Ra > Ra_{cr}$ .

#### 2 Statement of the problem on the Rayleigh–Bénard instability

The instability of a layer of liquid heated from below (the Rayleigh–Bénard instability) is due to the difference in densities of the upper and lower layers. Thermodynamically, this instability is consequent on the difference in the energy states of liquid particles forming a layer in the gravitational field. To assess the trends to liquid "separation" with the formation of macro- and meso-scale structures (convective cells, vortexes, turbulent moles), we shall be only concerned with the gravitation component of the total enthalpy. This component is the potential energy in the field of gravity forces, which for a liquid particle (of unit volume) is equal to  $\rho gx$  (x is the coordinate corresponding to the layer height,  $\rho$  is the density, g is the acceleration of gravity). The difference in temperatures is responsible for the difference in densities of the upper and lower layers. The dependence of the liquid density on temperature (the state equation with constant pressure P = const) reads as

$$\varrho = \frac{\varrho_*}{1 + \beta_T \left(T - T_*\right)} \tag{1}$$

 $(\varrho_*, T_* \text{ are parameters of the reference state})$ , where  $\beta_T$  is the thermal-expansion coefficient (which, for purposes of estimation, is assumed to be constant in some interval of temperatures; for water  $0.15 \cdot 10^{-3} \cdot K^{-1}$ , for oil  $0.7 \cdot 10^{-3} \cdot K^{-1}$ ). To fix the the reference system, we choose the upper layer of liquid, whose temperature is maintained constant, with parameters  $\varrho_*, T_*, x_*$ ; for the lower layer we have  $x = x_0 = 0$ ,  $T = T_0$ ; the control parameter is  $T_0$ .

Introducing the dimensionless density  $\left(\tilde{\varrho} = \frac{\varrho}{\varrho_*}\right)$  and the temperature  $\left(\tilde{T} = \frac{T}{T_*}\right)$ , this gives

$$\widetilde{\varrho} = \frac{1}{1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)} \tag{2}$$

where  $\widetilde{\beta} = \beta_T T_*$  is the dimensionless thermal-expansion coefficient ( $\widetilde{\beta}$  is estimated as follows:  $\beta_T \sim 0.7 \cdot 10^{-3} \cdot K^{-1}; T \sim 300 K \Rightarrow, \widetilde{\beta} \sim 0.2$ ).

The excessive enthalpy, which characterizes the energy inhomogeneity of a liquid layer, will be estimated as the difference with respect to the enthalpy of the layers close to the homogeneous state (the middle layer of the liquid). The excessive entropy of an inhomogeneous system will be written in the form of the entropy of a "perfect mixture" of liquid particles, which have different energy in the gravitational field. These two thermodynamic functions enable one to represent the free Gibbs energy (or the free Helmholtz energy, depending on the problem) with the help of the Gibbs–Helmholtz equation.

Another form of this representation is the Ginzburg–Landau potential, which as a rule as written in the form of a forth-degree polynomial. The graphs of the Ginzburg– Landau potential for the first and second cases have the same appearance. However, their principal difference is that *ab initio* the free Gibbs energy is constructed from the physical (thermodynamic) ideas, which, when formalized, give the "mathematical result"—the explicit form of the dependence. The Ginzburg–Landau potential is originally constructed by a formal decomposition into a series with retaining only terms of order four (or smaller). In this form, this representation becomes capable of describing instability phenomena (if a potential has one minimum, then the system is thermodynamically stable; if the potential has two minima and one maximum between them, then the system is thermodynamically unstable, and hence may feature processes like nonequilibrium phase transitions). Following the formal mathematical analysis, it is required to physically interpret the coefficients of this series (their signs and numerical values). However, as a rule, the main emphasis is usually placed on the mathematical part of a problem, leaving aside the physical interpretation.

With this proviso, below use will be made the representation of the Ginzburg– Landau potential in the Gibbs–Helmholtz form. In this potential, the enthalpy and entropy can be written not only in the form which describes the perfect system, but also the systems involving the interaction and some other statistics for entropy. However, to assess the capabilities of the approach, on the first step we should use the maximally "idealized" description.

As was already pointed out, such statement of the problem is capable of singling out the gravitation component from the total enthalpy, which is the potential energy of a liquid particle in a gravitational field. It is worth noting that such a statement of the problem is well known; for example, the problem of finding the sedimentation-diffusive distribution of gases in the atmosphere in their altitude. The equilibrium distribution of gases is consequent on two opposite trends of minimizing and maximizing the entropy they are realized, respectively, as the sedimentation and diffusion. In this problem, the free Helmholtz energy in the form of a sedimentation-diffusive potential controls the distributions of gases in height.

The above digression justifies the use of the thermodynamic approach in the Rayleigh– Bénard problem. Under this approach, one first assesses the possibility of the realization of a thermodynamic instability with the help of a criterion in the form of the Ginzburg–Landau potential. Further, one estimates the possibility of the realization of the "diffusion separation" of the original system (macro-inhomogenous, but microhomogenous) with the formation of meso- and macro-scale structures; here, use is made of theory of phase transitions with the involvement of the machinery originating in the theory of the Cahn–Hillard spinodal decomposition.

The thermodynamic approach towards the Rayleigh–Bénard, depending on the Cahn–Hillard formalism [34]-[43], does not assume the negation of the classical "mechanical" method. Under this approach, the "thermodynamic solution" of the problem in the framework of the theory of nonequilibrium phase transitions is used to study and illustrate the capabilities of the approach with the aim of later extension to other examples of evolution of unstable systems. For some such systems, according to [46] the approach of the continuum mechanics faces certain difficulties.

# 3 Construction of the Ginzburg–Landau potential for the Rayleigh–Bénard problem in the form of the free Gibbs– Helmholtz energy

According to [47], the distribution of the temperature over the body length (a bar, a liquid layer), whose boundaries are kept with constant different temperatures, is linear. Hence, for the distribution of the temperature in a layer of liquid, we shall assume in the Rayleigh–Bénard problem that

$$T(x) = T_* + (T_0 - T_*) \frac{x_* - x}{x_*}$$
(3)

where  $T_*$  is the (minimal) temperature of the upper layer,  $T_0$  is the (maximal) temperature of the lower layer (the control parameter),  $x_*$  is the height of the layer, x is the current coordinate over the layer height (on the lower "hot" side  $x = x_0 = 0$ ). The middle layer of liquid is sedimentation-neutral; the upper layer (with small temperature, and respectively, large density) is prone to positive sedimentation (subsidence), while the lower one (of large temperature and small density), is liable to negative sedimentation (floating). Both these layers (the upper and lower ones) feature excessive enthalpy (gravitation component) with respect to the middle layer; that is,

$$(\varrho_* - \varrho_m) g(x_* - x_m) > 0, \text{ here } (\varrho_* - \varrho_m) > 0, x_* - x_m > 0,$$
 (4)

$$(\varrho_0 - \varrho_m) g(x_0 - x_m) > 0$$
, here  $(\varrho_0 - \varrho_m) < 0, x_0 - x_m < 0$ , (5)

where  $\rho_m x_m$  is the density and coordinate of the middle layer.

For each local layer of liquid, the gravitation component of enthalpy can be written in form

$$H_g = (\varrho - \varrho_m) g(x - x_m).$$
(6)

Using dependences (1) and (2), the enthalpy can be represented as a function of the temperature. The process of formation of an inhomogeneous state of a liquid layer is known to take place with supply of heat, and hence the enthalpy of this (endothermic) process is positive in accordance with the thermodynamic sign system. In the large, in the framework of the theory of nonequilibrium phase transitions, the process of formation of inhomogeneous liquid and subsequent "decomposition" into convective cells will correspond to the phase decomposition process in systems with lower critical decomposition point (the variations of the enthalpy and entropy during the process are positive).

At this point, we need some calculations.

1)

$$T_m = \frac{1}{2} \left( T_0 + T_* \right) = T_* \ \widetilde{T}_m. \ \widetilde{T}_m = \frac{1}{2} \left( \frac{T_0}{T_*} + 1 \right) = \frac{1}{2} \left( \widetilde{T}_0 + 1 \right)$$
(7)

where  $\widetilde{T}_0 = T_0/T_*, \ \widetilde{T} = T/T_*, \ 1 < \widetilde{T} < \widetilde{T}_0;$ 

2)

$$\varrho - \varrho_m = \varrho_* \left( \frac{1}{1 + \widetilde{\beta} \left( \widetilde{T} - 1 \right)} - \frac{2}{2 + \widetilde{\beta} \left( \widetilde{T}_0 - 1 \right)} \right)$$

3) we express the x-coordinate in terms of  $\widetilde{T}$ . Using (3), we find that

$$\widetilde{T} = 1 + \left(\widetilde{T}_0 - 1\right)\left(1 - \widetilde{x}\right) \tag{8}$$

and so

$$\widetilde{x} = 1 - \frac{\widetilde{T} - 1}{\left(\widetilde{T}_0 - 1\right)} \tag{9}$$

4)

$$x - x_m = x_* \left( \widetilde{x} - \widetilde{x}_m \right) = x_* \left( \widetilde{x} - \frac{1}{2} \left( 1 + \widetilde{x}_0 \right) \right) = \frac{1}{2} x_* \left( 1 - \frac{2\left( \widetilde{T} - 1 \right)}{\left( \widetilde{T}_0 - 1 \right)} \right)$$
(10)

Let us introduce the dimensionless parameter for the gravitation component of the enthalpy  $H_*$ :

$$H_{*} = (\varrho_{*} - \varrho_{m}) g(x_{*} - x_{m}) = x_{*}\varrho_{*} (1 - \tilde{\varrho}_{m}) g(1 - \tilde{x}_{m}) = \frac{1}{4}x_{*}g\varrho_{*} (1 - \tilde{\varrho}_{0}) (1 - \tilde{x}_{0}) =$$
(11)
$$= \frac{1}{4}x_{*}g\varrho_{*} \left(1 - \frac{2}{2 + \tilde{\beta}\left(\tilde{T}_{0} - 1\right)}\right)$$

(here, g is the acceleration of gravity). As a result, for the dimensionless enthalpy  $h\left(\widetilde{T}\right)$  we have by (6) and (11)

$$h\left(\tilde{T}\right) = \frac{H_g}{H_*} = \frac{\left(\tilde{\varrho} - \tilde{\varrho}_m\right) g \left(\tilde{x} - \tilde{x}_m\right)}{\left(1 - \tilde{\varrho}_m\right) g \left(1 - \tilde{x}_m\right)} =$$
(12)  
$$= \frac{\left(\frac{1}{1 + \tilde{\beta}(\tilde{T} - 1)} - \frac{2}{2 + \tilde{\beta}(\tilde{T}_0 - 1)}\right) \left(1 - \frac{\tilde{T} - 1}{(\tilde{T}_0 - 1)} - \frac{1}{2}\left(1 + \tilde{x}_0\right)\right)}{\left(1 - \frac{2}{2 + \tilde{\beta}(\tilde{T}_0 - 1)}\right) \left(1 - \frac{1}{2}\left(1 + \tilde{x}_0\right)\right)} =$$
$$= \frac{\left(\frac{1}{1 + \tilde{\beta}(\tilde{T} - 1)} - \frac{2}{2 + \tilde{\beta}(\tilde{T}_0 - 1)}\right) \left(1 - \frac{2(\tilde{T} - 1)}{(\tilde{T}_0 - 1)}\right)}{\left(1 - \frac{2}{2 + \tilde{\beta}(\tilde{T}_0 - 1)}\right)}$$

As was already pointed out, the energy inhomogeneity of a system can be assessed, using the expression for the entropy of a perfect mixture, as the inhomogeneity of

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a "perfect" mixture of energetically various particles. Each local liquid layer being characterized by the enthalpy, we have for the entropy

$$s\left(\widetilde{T}\right) = -[h\ln h + (1-h)\ln(1-h)] \tag{13}$$

the Gibbs–Helmholtz potential in the form of the free Gibbs–Helmholtz energy reading as

$$g\left(\widetilde{T}\right) = h\left(\widetilde{T}\right) - \gamma\left(\widetilde{T}\right)s\left(\widetilde{T}\right)$$
(14)

where  $\gamma\left(\widetilde{T}\right)$  is an analogue of the temperature for the gravitation component of the enthalpy. This quantity can be represented in the form  $\gamma\left(\widetilde{T}\right) = h\left(\widetilde{T}\right)/\alpha\left(\widetilde{T}\right)$ , where  $\alpha\left(\widetilde{T}\right)$  is the energy capacity of an energetically inhomogeneous system (an analogue of the differential heat capacity, which decreases with increasing temperature). The propensity of a system to convective mixing increases with increasing temperature (that is, the contribution of the "supramolecular" entropy component (which may be called configurational) increases, and hence the parameter  $\mu\left(\widetilde{T}\right) = 1/\alpha\left(\widetilde{T}\right)$  must increase with increasing temperature. With this representation (14) reads as

$$g\left(\widetilde{T}\right) = h\left(\widetilde{T}\right) - \mu\left(\widetilde{T}\right)h\left(\widetilde{T}\right)s\left(\widetilde{T}\right)$$
(15)

where  $\mu\left(\widetilde{T}\right)$  is an increasing function.

Here, we observe the following trends and analogies:  $\Delta H = c_p T$  ( $c_p$  is the isobaric heat capacity),  $T = \Delta H/c_p$ , that is,  $\gamma\left(\widetilde{T}\right)$  is an analogue of  $T, \alpha\left(\widetilde{T}\right)$  is an analogue of  $c_p$ ; with increasing T the differential heat capacity  $\Delta c_p (\partial c_p / \partial T)$  decreases; that is, the following trends should be manifested with increasing  $\widetilde{T}$ : a growth in  $\widetilde{T}$  reduces  $\alpha\left(\widetilde{T}\right)$ , and correspondingly, a growth in  $\widetilde{T}$  increases  $1/\alpha\left(\widetilde{T}\right)$  and  $\mu\left(\widetilde{T}\right)$ .

For the purposes of matching dimensions and introducing substantiated numerical values of characteristic parameters, we shall estimate the order of some quantities.

To estimate  $H_g$  we shall put  $\rho_* \sim 1 \cdot 10^3 \text{kg/m}^3 \ g \sim 10 \text{m/s}^2$ ,  $x_* \sim 1 \cdot 10^{-2} \text{m}$ . Now

 $x_*g\varrho_*$  is of the order  $\sim 1 \text{J/m}^3$  or  $x_*g\varrho_* \sim 1 \cdot 10^{-3} \text{J/kg}^3$ . To match the orders of  $h\left(\widetilde{T}\right), s\left(\widetilde{T}\right)$  and  $g\left(\widetilde{T}\right)$ , we shall assume that a part of liquid of continuum mechanics (in the case of liquid) has linear size of order  $d \sim$  $0.1-1\mu m$ ;  $(1\cdot 10^{-7}-1\cdot 10^{-5}m)$ . Thus, for  $d\approx 0.2\mu m$  for the parameter  $RT_*$  (the factor multiplying the entropy term), we have  $RT_* \sim 1 \text{J/m}^3$ , the conditional molecular mass of a part of liquid of continuum mechanics being of order  $\sim 1 \cdot 10^9$  g/mole (the molecular mass of the Prandtl mole). In this case,  $h\left(\widetilde{T}\right)$ ,  $s\left(\widetilde{T}\right)$  and  $g\left(\widetilde{T}\right)$  are commensurable.

For a qualitative analysis of how well the above expressions predict the behavior of the system in the Rayleigh–Bénard problem, we shall introduce a new dimensionless variable, which is the variation of the temperature. Since the above dimensionless temperature  $\tilde{T}$  varies in the range from 1 to  $\tilde{T}_0$ ,  $(1 < \tilde{T} < \tilde{T}_0)$ , we introduce the variable 
$$\begin{split} \theta &= \frac{\widetilde{T}-1}{\widetilde{T}_0-1} \text{ with the range } 0 < \theta < 1 \text{ (since } 1 < \widetilde{T} < \widetilde{T}_0 \text{, we have } 0 \leq \widetilde{T}-1 < \widetilde{T}_0-1 \text{ and} \\ 0 &< \frac{\widetilde{T}-1}{\widetilde{T}_0-1} \leq 1 \text{, and hence } \theta = \frac{\widetilde{T}-1}{\widetilde{T}_0-1} \text{).} \\ \text{Let us rewrite the above expressions } qua \text{ functions of } \theta : \\ 1 \text{)} \end{split}$$

$$\widetilde{\varrho} = \frac{1}{1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)} = \frac{1}{1 + \widetilde{\beta}\left(\widetilde{T}_0 - 1\right)\theta}$$
(16)

2)

$$\widetilde{x} = 1 - \frac{\widetilde{T} - 1}{\widetilde{T}_0 - 1} = 1 - \theta 3$$
(17)

3)

$$\varrho - \varrho_m = \varrho_* \left( \frac{1}{1 + \widetilde{\beta} \left( \widetilde{T} - 1 \right)} - \frac{2}{2 + \widetilde{\beta} \left( \widetilde{T}_0 - 1 \right)} \right) =$$

$$= \varrho_* \left( \frac{1}{1 + \widetilde{\beta} \left( \widetilde{T}_0 - 1 \right) \theta} - \frac{2}{2 + \widetilde{\beta} \left( \widetilde{T}_0 - 1 \right)} \right)$$
(18)

(4)

$$x - x_m = x_* \left( \widetilde{x} - \widetilde{x}_m \right) = \frac{1}{2} x_* \left( 1 - \frac{2\left( \widetilde{T} - 1 \right)}{\left( \widetilde{T}_0 - 1 \right)} \right) = \frac{1}{2} x_* \left( 1 - 2\theta \right)$$
(19)

5)

$$h\left(\theta\right) = \frac{\left(\frac{1}{1+\tilde{\beta}\left(\tilde{T}_{0}-1\right)\theta} - \frac{2}{2+\tilde{\beta}\left(\tilde{T}_{0}-1\right)}\right) \quad (1-2\theta)}{\left(1 - \frac{2}{2+\tilde{\beta}\left(\tilde{T}_{0}-1\right)}\right)} \tag{20}$$

6)

$$s(\theta) = -[h(\theta)\ln h(\theta) + (1 - h(\theta))\ln (1 - h(\theta))]$$
(21)

7)

$$g(\theta) = h(\theta) - \mu(\theta) h(\theta) s(\theta)$$
(22)

In the Rayleigh–Bénard problem, for small gradient of the temperature over the liquid layer, the system remains convection-stable; that is, for small gradients of the temperature, the heat conduction manages to transform the heat energy from the source to the sink. For large gradients of the temperature, the heat conduction mechanism is incapable of transmitting large amounts of energy, and the system "switches" to a different (convective) mechanism. Furthermore, for small gradients of the temperature, the stability of the system can be reconstructed by introducing the stabilizing factor (the "molecular" component of the entropy); in this case, the stability is secured by the heat conduction, and hence the entropy of a thermally-inhomogeneous system, *qua* an "ideal" mixture, can be represented in the form

$$\varphi(\theta) = -[\theta \ln \theta + (1 - \theta) \ln (1 - \theta)]. \tag{23}$$

The trend of the system to a thermally homogeneous state is provided by the heat conduction—the more intense is this trend, the smaller is the trend to the realization of the convective mixing; that is, these two trends are oppositely directed. Hence, the contribution of the "molecular" component of the entropy into the free energy can be written in the form

$$\psi\left(\theta\right) = \eta\left(\theta\right)\theta\varphi\left(\theta\right),\tag{24}$$

where the parameter  $\eta(\theta)$  is an analogue of  $\mu(\theta)$  in (15).

Thus, in view of the two trends trends for realization of (molecular and convective) mixing, the Ginzburg–Landau potential in the Gibbs–Helmholtz form can be written as

$$f(\theta) = h(\theta) - \mu(\theta) h(\theta) s(\theta) + \psi(\theta)$$
(25)

Besides, instead of the dependence  $\psi(\theta)$  (24) for the study of the qualitative behavior, one may consider the dependence

$$\omega\left(\theta\right) = \eta\left(\theta\right) \cdot \varphi\left(\theta\right) \tag{26}$$

which for the Ginzburg–Landau potential gives a representation similar to (25),

$$z(\theta) = h(\theta) - \mu(\theta) h(\theta) s(\theta) + \omega(\theta)$$
(27)

Illustrations of the dependences  $g(\theta)(22)$ ,  $f(\theta)$  from (25) and  $z(\theta)$  from (27) are given in Fig. 1; for the purposes of the qualitative analysis of the behavioral trends of the system, the parameters  $\mu$  and  $\eta$  are taken to be constants, considering that these parameters increase with increasing temperature.

The dependence  $g(\theta)$  from Fig. 1.a suggest that the following scenario for the instability of a liquid layer heated from below can be realized. In regions where  $g(\theta) < 0$  the liquid layers are unstable with respect to the convective mixing. These are the regions lying below or above the middle layers. In the middle layers  $g(\theta) > 0$ , and here, the perturbations must die down. Hence, in case there develops the motion of upper layers down and lower layers up due to increasing perturbations in them, the middle layers, which remain stable, can be viewed as conditionally "monolithic formations". These "monolithic formations" may move as a whole; that is, they may be taken by adjacent flows without considerable relative displacements inside the layer. Perturbations in such layers die dow, and hence the intensity of such displacements of such kind must sharply decrease from the edge of the layer to its center.



Figure 1: The dependences  $g(\theta)$  (22),  $f(\theta)$  (25) and  $z(\theta)$  (27) with  $\tilde{\beta} = 0.2$ ;  $\tilde{T}_0 = 2.0$ ;  $\mu(\theta) = \text{const} = 2.0$ ;  $\eta(\theta) = \text{const} = 0.2$ ;  $\chi(\theta) = 0$  fixes the zero level.

Considering the behavior of the dependence  $g(\theta)$  from the left maximum downwards to the left minimum, it follows that the inflection of the curve  $\frac{d^2}{d\theta}^2 g(\theta) < 0$  lies in the region where  $g(\theta) < 0$ . This means that in the region where  $\frac{d^2}{d\theta}^2 g(\theta) < 0$  (to the right of the inflection point) the liquid layers are in the labile zone (that is, they are unstable with respect to infinitely small perturbations). Hence, one may suppose hat these layers are "generators" of the perturbations. The layers with  $\frac{d^2}{d\theta^2}g(\theta) > 0$  are in the region of metastability, and hence they are unstable against perturbations that exceed certain critical level (analogue of the Gibbs nucleus in the theory of nonequilibrium phase transitions), which will increase, forming a steady convective flow. It may be also supposed that the perturbations generated in the labile zone of these layers will be external with respect to such layers. Besides, the perturbations generated in the labile zone will become more and more intense until reaching a sufficiently high level, which may secure the development of the instability also in the metastable region.

This system has one significant peculiarity: the labile zones (lower and upper) are directly adjacent not only with metastable regions, but also with stable regions (middle layers). Such a situation is not peculiar to the nonequilibrium phase transitions, where labile zones are adjacent only with metastable regions. This peculiarity is due to the "geometric" nature of the problem. in which upper and lower layers (with respect to the central ones) are unstable.

The introduction of the correction to a possibly partial thermal decrease of the inhomogeneity (the representation of the Ginzburg–Landau potential in the form  $f(\theta)$  (25), see Fig. 1.b, or  $z(\theta)$  (27), Fig. 1.c) has no principal effect on the qualitative behavior of the system. The system, as one may expect, becomes more stable, to a certain degree, with respect to the convection.

Considering the setting of Fig. 1 as an example, one may note that a decrease in the gradient of the temperature in the large over the liquid layer may make the system unstable with respect to the convection:  $g(\theta) > 0$  for all layers of liquid (Fig. 2). An increase of the gradient of temperature in the large over the liquid layer (Fig. 3) has an opposite effect: the regions with convection-stable layers become more narrow, while the regions with unstable layers are expanding.

It is also worth noting that the dependence (22) is asymmetric — this is because, first of all, the dependence of density on the temperature. This asymmetry unveils the fact that the upper layers near the "cold" surface are more stable than the lower ones



Figure 2: The dependences  $g(\theta)$  (22) and  $f(\theta)$  (25) with  $\tilde{\beta} = 0.2$ ;  $\tilde{T}_0 = 1.2$ ;  $\mu(\theta) = \text{const} = 1.2$ ;  $\eta(\theta) = \text{const} = 0.1$ ;  $\chi(\theta) = 0$  fixes the zero level.



Figure 3: The dependences  $g(\theta)$  (22) and  $f(\theta)$  (25) with  $\tilde{\beta} = 0.2$ ;  $\tilde{T}_0 = 3.0$ ;  $\mu(\theta) = \text{const} = 3.0$ ;  $\eta(\theta) = \text{const} = 0.3$ ;  $\chi(\theta) = 0$  fixes the zero level.

near the "hot" surface.

The above scenario for convective instability is only anticipated, because it is based only on the thermodynamic representation of a system (that is, on its potential (intrinsic) capabilities). At the same time, the thermodynamics acknowledges that there is a possibility of stratification of an initially "convectively" homogeneous system into convective cells (Bénard cells). In the large, the development of a convective instability is also governed by the "kinetic" properties of a system (that is, by the character of the development of perturbations in time).

Within the approach of [30], [50] to the description of nonequilibrium phase transitions, these properties are consequent to the intensity of the processes, which are conventionally called "negative" diffusion. Earlier it was shown that such an approach may also be extended to the laminar-turbulent transition [30]. In the present paper, this approach is tested on the well-known Rayleigh–Bénard instability problem. It turned out that, for this problem, the Ginzburg–Landau potential has the same distinctive features as for the laminar-turbulent transition problem. The principal differences are in the "geometry" of systems.

The principal trends in the change of the functions  $g(\theta)$  (22),  $f(\theta)$ (25) and  $z(\theta)$ (27) with variation of the parameters  $\mu(\theta)$  and  $\eta(\theta)$  are as follows.

An increase in  $\mu(\theta)$  (with  $\eta(\theta) = \text{const}$ ) results in a transition from the stability state to the state of instability. This transition corresponds to the bifurcation value of the parameter  $\mu(\theta)$ , for example, for  $g(\theta)$  for  $\eta(\theta) = 0.2$ ,  $\tilde{T}_0 = 2$ ,  $\tilde{\beta} = 0.2$  this value is  $\mu_{\text{cr}}^* = 1.45$ ; that is, this parameter is an analogue of the Rayleigh number in the classical problem of the Rayleigh–Bénard instability.

An increase in  $\eta(\theta)$  for  $\mu(\theta) = \text{const results}$  in the "suppression of instability"—the zone of stratification-stable layers expands, a higher value of the parameter  $\eta(\theta)$  gives a larger value of  $\mu_{\text{cr}}^*$ .

Thus, the parameter  $\eta(\theta)$  is capable of elucidating the trends of the contribution from the molecular component on maintaining the thermal homogeneity of the system. In this respect, the parameter  $\eta(\theta)$ , as well as the parameter  $\mu(\theta)$ , determines the trends, which in the classical statement of the problem are represented by the Rayleigh number  $Ra = \frac{g\beta\Delta TL^2}{\nu\lambda}$  (here, g is the acceleration of gravity,  $\beta$  is the thermal-expansion coefficient of liquid,  $\Delta T$  is the difference between the temperatures between the "hot" and "cold" walls, L is the characteristic linear size (the height of the heated layer of liquid),  $\nu$  is the kinematic viscosity of liquid,  $\lambda$  is the thermometric conductivity of liquid), namely, the parameter  $\eta(\theta)$  is determined by the viscosity and heat conduction. These trends can be written as  $\eta(\theta) \sim \nu\lambda$ ; that is, the large value of  $\lambda$  promotes the leveling of the thermal inhomogeneity, thereby hindering the onset of convective instability. The high value of  $\nu$  also impedes the instability, but because of the different mechanism. If a growth of  $\lambda$  is responsible for a decrease in the gradient of the temperature over the liquid layer (thereby stabilizing it), then the growth of  $\nu$  has no effect on the gradient of the temperature, but increases that value thereof which is necessary for a transition to the state of instability with respect to the convection.

This being so, the classical Rayleigh test splits into two criteria:  $\mu(\theta)$  and  $\eta(\theta)$ , where  $\mu(\theta) \sim Ra_1$  and  $\eta(\theta) \sim 1/Ra_2$ , which track the states of an inhomogeneous liquid in the macro- (meso-) and micro-level, respectively.

### 4 Analysis of thermodynamic relations for the Rayleigh–Bénard problem

As was pointed out above, the global inhomogeneity of a system can be looked upon as an inhomogeneity of the enthalpy distribution over the height of the liquid. In view of the gravitational component, this equation can be put in the form [51]

$$dW - TdS + PdV - \varrho g dx = d \left(W - TS - \varrho g x\right) +$$

$$+SdT - \frac{P}{\rho^2} d\varrho + g x \ d\varrho$$
(28)

here, we used the fact that  $P \, dV = P \, d\left(\frac{1}{\varrho}\right) = -\frac{P}{\varrho^2} d\varrho$ , where x is the coordinate in the liquid height,  $\varrho$  is the density, g is the acceleration of gravity, W is the internal energy,  $-\varrho g \, dx$  is the gravitational part of the internal energy. The quantity  $T dS + \varrho g dx$  may be interpreted as a supplement to the internal energy (enthalpy) due to the system inhomogeneity (in density and temperature). The sum of the four terms in (28) is the total differential for a local equilibrium state (for a specific state of the system the total energy  $\mathcal{E}$  is constant). The additional "capacity" of energy of an inhomogeneous system can be characterized by the quantity of the form

$$dS + \frac{\varrho g}{T} dx \tag{29}$$

(an analogue of the heat capacity for a homogeneous system). It can be assumed that this quantity serves as a criterion for the transition from the region of molecule heat conduction to the regime of convective heat conduction, because the "capacity" of liquid for the energy (qua a molecular system) can be exceeded.

The Rayleigh–Bénard problem is a classical problem to verify and tune various methods of solution. Besides, various approaches tested on this problem enable one to better visualize various physical aspects of the phenomenon of Rayleigh–Bénard instability, as well as others, which can be subsumed into the class of nonequilibrium phase transitions. For example, in [52] one distinctive feature is pointed out: "... the stationary state corresponds to the minimal entropy... However, the situation changes as soon as the instability threshold is crossed. Bénard vortexes produce more entropy than it follows from the theorem of minimum entropy production". Thus, one may say that the quantity in (29) characterizes the situation when the production of the entropy higher than in the case of the molecule heat conduction. Since according to Boltzmann the entropy is a "structure-sensitive" function, it follows that it is the quantity in (29) that characterizes the structural transformation of a system or a nonequilibrium phase transition.

For local states, we introduce the dimensional relative quantities

$$\widetilde{\varepsilon}_B = g\varrho_* x_* / W_*, \ \widetilde{W} = W / W_*, \ \widetilde{S} = S / S_*; \ \widetilde{P} = P / P_*, \ W_* = S_* T_*,$$
(30)

here,  $\tilde{\varepsilon}_B$  is the dimensionless local gravitation component of the enthalpy. Hence, by (2) equation (28) can be put the form

$$\frac{1}{W_*} \left( dW - TdS + PdV - \varrho g dx \right) =$$

$$= d \left( \widetilde{W} - \widetilde{T}\widetilde{S} - \frac{1}{\left( 1 + \widetilde{\beta} \left( \widetilde{T} - 1 \right) \right)} \widetilde{\varepsilon}_B \widetilde{x} \right) + \frac{1}{W_*} \left( SdT - \frac{P}{\varrho^2} d\varrho + gx \, d\varrho \right);$$
(31)

here,

$$\frac{1}{W_*} \left( SdT - \frac{P}{\varrho^2} d\varrho + gx \, d\varrho \right) = \left( \widetilde{S} + \widetilde{\beta} \widetilde{P} - \widetilde{\beta} \widetilde{\varepsilon}_B \widetilde{x} \, \frac{1}{\left( 1 + \widetilde{\beta} \left( \widetilde{T} - 1 \right) \right)^2} \right) d\widetilde{T} \qquad (32)$$

We shall require that

$$\widetilde{S} + \widetilde{\beta}\widetilde{P} - \widetilde{\beta}\widetilde{\varepsilon}_B\widetilde{x} \frac{1}{\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)^2} = 0$$
(33)

(this requirement is equivalent to the realization of a local equilibrium). As a result, we have

$$\widetilde{P} = -\frac{1}{\widetilde{\beta}} \left( \widetilde{S} - \widetilde{\beta} \widetilde{\varepsilon}_B \widetilde{x} \frac{1}{\left(1 + \widetilde{\beta} \left(\widetilde{T} - 1\right)\right)^2} \right).$$
(34)

This relation determines the local equilibrium manifold in the phase space, on which the increment of the enthalpy

$$\frac{1}{W_*} \left( dW - TdS - PdV - \varrho g dx \right) =$$

$$= d \left\{ \widetilde{W} - \widetilde{T}\widetilde{S} - \widetilde{\varepsilon}_B \left( \frac{1}{\left( 1 + \widetilde{\beta} \left( \widetilde{T} - 1 \right) \right)} \widetilde{x} - 1 \right) \right\}$$

$$(35)$$

is a total differential; here,

$$\left(\widetilde{W} - \widetilde{T}\widetilde{S}\right)\Big|_{\widetilde{T} = \widetilde{T}_* = 1, \widetilde{S} = \widetilde{S}_* = 1, \widetilde{W} = \widetilde{W}_* = 1} = 0, \quad \frac{1}{\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)}\widetilde{x}\Big|_{\widetilde{T} = \widetilde{T}_* = 1, \widetilde{x} = \widetilde{x}_* = 1} = 1.$$
(36)

Thus, the system of state equations

$$\widetilde{\varrho} = \frac{1}{1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)}, \quad \widetilde{P} = -\frac{1}{\widetilde{\beta}}\left(\widetilde{S} - \widetilde{\beta}\widetilde{g}\widetilde{x} \frac{1}{\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)^2}\right)$$
(37)

determines in the phase space the local equilibrium manifold, on which the left-hand side of (35) is a total differential.

## 5 Gravitation-convection potential for thermodynamic systems featuring the Rayleigh–Bénard instability

In analogy with [50], we shall introduce the relative quantities: enthalpy, entropy, and the free Gibbs energy. To this aim, we first introduce the analogue of the turbulization parameter [50] (the order parameter [28]), *viz.*, the parameter of convection production

$$\xi^2 = \frac{\widetilde{W} - \widetilde{T}\ \widetilde{S}}{\widetilde{T}\ \widetilde{S}} \tag{38}$$

for a process with excess energy

$$\widetilde{W} - \widetilde{T} \ \widetilde{S} > 0 \tag{39}$$

We define the relative quantity, which is the total contribution of the gravitationconvection component in the enthalpy with excess energy, as follows:

$$h\left(\xi\right) = \frac{\widetilde{W} - \widetilde{T}\widetilde{S} - \widetilde{\varepsilon}_{B}\left(\frac{1}{\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)}\widetilde{x} - 1\right)}{\widetilde{T}\widetilde{S}} = \xi^{2} - \frac{\widetilde{\varepsilon}_{B}\left(\widetilde{x} - 1 - \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)}{\widetilde{T}\widetilde{S}\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)}; \quad (40)$$

the dimensional quantity

$$\nu_B = \frac{\widetilde{\varepsilon}_B \left( \widetilde{x} - 1 - \widetilde{\beta} \left( \widetilde{T} - 1 \right) \right)}{\widetilde{T} \widetilde{S} \left( 1 + \widetilde{\beta} \left( \widetilde{T} - 1 \right) \right)}$$
(41)

will be called the Bénard number. Now (40) can be put in the form

$$h\left(\xi\right) = \xi^2 - \nu_B. \tag{42}$$

Note that for  $\widetilde{T} > 1$  (the superheat condition) we have  $\nu_B < 0$ 

The entropy and the free Gibbs energy will be defined as follows:

$$s(\xi) = -(\xi^{2} - \nu_{B}) \ln(\xi^{2} - \nu_{B}) - (1 + \nu_{B} - \xi^{2}) \ln(1 + \nu_{B} - \xi^{2})$$
$$g(\xi) = h(\xi) - \alpha h(\xi) s(\xi);$$

here,

$$\nu_B < \xi^2 < 1 + \nu_B$$

Now

$$g(\xi) = (\xi^2 - \nu_B) - (43) -\alpha (\xi^2 - \nu_B) \left[ -(\xi^2 - \nu_B) \ln (\xi^2 - \nu_B) - (1 + \nu_B - \xi^2) \ln (1 + \nu_B - \xi^2) \right].$$

In the case, when the superheat condition  $\widetilde{T} > 1$  is satisfied (that is,  $\nu_B < 0$ ), the structure of the relative enthalpy, entropy, and the free Gibbs energy is the same as in [50] for the laminar-turbulent transition:

$$h(\xi) = \xi^{2} + |\nu_{B}|,$$

$$s(\xi) = -(\xi^{2} + |\nu_{B}|) \ln(\xi^{2} + |\nu_{B}|) - (1 - |\nu_{B}| - \xi^{2}) \ln(1 - |\nu_{B}| - \xi^{2}),$$

$$g(\xi, |\nu_{B}|) = h(\xi) - \alpha h(\xi) s(\xi)$$

$$(44)$$

Experiments show that a turbulent flow has lamellar structure with interlacing zones of large and small turbulization (see [35], [36]). The same structure features the Rayleigh–Bénard convective instability. For a potential  $g(\xi)$  which is symmetric about  $\xi = 0$ , the pump of the internal energy due to the Cahn–Hillard operator on the right of the fourth equation in (58) is determined by the support tangent (that is, by the negative minima  $((\xi^{\pm}, g(\xi^{\pm})))$  of the potential  $g(\xi)$ , where  $\xi^{-} = -\xi^{+}$ ). This determines the amplitudes  $|\xi(x,t)|$  of the same nature in the neighboring regions of the lamellar structure of the solution, which disturbs the interlace of zones with large and small convection production. Besides, in the first approximation, the boundaries of the lamellar zones do not move. These facts call for the following correction of the dependence of the free energy (in analogy with [50])

$$\widetilde{g}(\xi) = \begin{cases} g(\xi, |\nu_B|), & \xi > 0\\ \gamma \xi^2 \left( 1 + \alpha \left( 1 - \xi^2 \right)^6 \ln \left( 1 - \xi^2 \right) \right) + g(0), & \xi < 0 \end{cases}$$
(45)

where  $\gamma$  is chosen from the condition

$$\frac{d^2}{d\xi^2}(\xi^2(1+\alpha(1-\xi^2)^6\ln(1-\xi^2))(0) = g''(0).$$



Figure 4: (a) Potential in the form of free energy  $\hat{g}$  for  $|\nu_B| = 0.2, \alpha = 0.5, 0.6, 0.7, 0.8$ ; (b) Potential in the form of free energy  $\hat{g}$  for  $|\nu_B| = 0.2, \alpha = 0.9, 1, 1.1, 1.2$ .; (c) Potential in the form of free energy  $\hat{g}$  for  $|\nu_B| = 0.05, \alpha = 1.3, 1.4, 1.5, 1.6$ ; (d) Potential in the form of free energy  $\hat{g}$  for  $|\nu_B| = 0.05, \alpha = 1.7; 1.8; 1.9; ; 2.0$ .

Let us give the dependence of the graphs  $\tilde{g}(\xi)$  on  $\alpha = 0.05, \ldots, 2.0$  with fixed  $\beta = 0.5; 0.2; 0.1; 0.05; 0.01$ . These dependences are illustrated in Figs. 4a–4f in the form of dimensionless variables.

>From the following five points  $(|\nu_B| = 0.5, \alpha = 0.4), (|\nu_B| = 0.2, \alpha = 0.6), (|\nu_B| = 0.1, \alpha = 1.2), (|\nu_B| = 0.05, \alpha = 1, 6), (|\nu_B| = 0.01, \alpha = 2)$  we construct the function  $\alpha = \alpha$  ( $\beta$ ). Substituting the so-constructed  $\alpha$  ( $\beta$ ) into (45), we get the potential  $\hat{g}_B^{(1)}(\xi, |\nu_B|)$ . The graphs of the resulting potential  $\hat{g}_B^{(1)}$  are as follows.



Figure 5: Sections of the graph of the resulting potential  $\hat{g}_B^{(1)}$ : (a) for  $|\nu_B| = 0.36$ ; 0.31; 0.26; 0.21; (b) for  $|\nu_B| = 0.26$ ; 0.21; 0.16; 0.11; 0.06; 0.01.

## 6 To the construction of the Rayleigh–Bénard model for convective instability as an nonequilibrium phase transition

The above construction illustrates the fact that the thermodynamic method is capable of ascertaining possible evolutions of a system—in this particular case, the trend for delamination into convection-stable and convection-unstable layers of liquid. It is worth noting that the above thermodynamic analysis is capable of not only determining the tendencies for the development of the convection-transition process (that is, a possibility of such a realization). At the same time, the choice of a trajectory and rate of evolution of the system depend on the kinetics of the instability process.

This being so, the thermodynamic analysis allows one to conclude that, in a layer of liquid heated from below, regions of stable and unstable states appear due to the inhomogenous distribution of density in the gravitational field. Unstable states are analogues of metastable and labile states in the theory of nonequilibrium phase transitions. This does not mean, however, that in stability regions no traces of convection will be observed with its developed state—the thing is that in these regions they will be eroded by the diffusion of perturbations, whereas in the instability regions (especially, in the labile region), the process of the "negative" (Cahn) diffusion will concentrate them. It can be assumed that the (convection)-instability regions of an originally homogeneous system are sources of perturbations (while the stability regions are sinks).

All these assumptions can be verified by a numerical experiment involving the mathematical model to be given below, which contains, in addition to the hydrodynamic equation (originally given in the most simple form), the mathematical model of nonequilibrium phase transition, as formulated in terms of the theory of Cahn–Hillard spinodal decomposition. This mathematical model of the Rayleigh–Bénard convective instability, considered as an analogue of a nonequilibrium phase transition, may become more involved, starting from the original thermodynamic model. As in [50], in simulating the Rayleigh–Bénard convective instability, we shall formulate three phenomenological hypotheses: this process is (1) the process of evolution of the system with excess energy and is (2) a nonequilibrium phase transition, governed by the mechanism of (3) diffusion separation. The process of diffusion separation into potentially convectively-stable and convectively-unstable layers of liquid further develops from the formation of a convective flow and can be represented within the formalism of continuum mechanics (in the simplest illustrative variant, this is a system of Euler equations). In this case, we start from the system of equations

$$\varrho \frac{d}{dt}T - \frac{\varrho_*}{\beta} \operatorname{div} U = 0,$$

$$\varrho \frac{d}{dt}U + \nabla P = \varrho g,$$

$$\varrho \frac{d}{dt}W + P \operatorname{div} U = 0,$$

$$\varrho \frac{d}{dt}S + \nu T^{\frac{\gamma}{\gamma - 1}} e^{-\kappa S} \operatorname{div} U = 0,$$
(46)

assuming that the state equations

$$\rho = \frac{1}{1 + \beta (T - 1)}, \quad P = -\frac{1}{\beta} \left( S - \beta g x \; \frac{1}{(1 + \beta (T - 1))^2} \right) \tag{47}$$

hold, where W is the internal energy, S is the macro entropy,  $\frac{d}{dt}F = \partial_t F + (U \cdot \partial_x) F$ . Using the first and fourth equations of (46), we have

$$\varrho \frac{d}{dt} \left( TS \right) + \left( -\frac{\varrho_*}{\beta} S + \nu T^{\frac{2\gamma - 1}{\gamma - 1}} e^{-\kappa S} \right) \, \operatorname{div} U = 0 \tag{48}$$

We set Q = TS. Hence,

$$\varrho \frac{d}{dt}Q + \left(-\frac{\varrho_*}{T\beta}Q + \nu T^{\frac{2\gamma-1}{\gamma-1}}e^{-\frac{\kappa}{T}Q}\right) \operatorname{div} U = 0$$
(49)

and so,

$$\varrho \frac{d}{dt}T - \frac{\varrho_*}{\beta} \operatorname{div} U = 0,$$

$$\varrho \frac{d}{dt}U + \nabla P = \varrho g,$$

$$\varrho \frac{d}{dt}Q + \left(-\frac{\varrho_*}{T\beta}Q + \nu T^{\frac{2\gamma-1}{\gamma-1}}e^{-\frac{\kappa}{T}Q}\right) \operatorname{div} U = 0,$$

$$\varrho \frac{d}{dt}(W - TS) + \left(P + \frac{\varrho_*}{\beta}S - \nu T^{\frac{2\gamma-1}{\gamma-1}}e^{-\kappa S}\right) \operatorname{div} U = 0,$$
(50)

In the dimensionless variables

$$x_{*} = U_{*}t_{*}, \ W_{*} = T_{*}S_{*}, \ P_{*} = \varrho_{*}U_{*}^{2}, \ S_{*}T_{*} = U_{*}^{2},$$

$$\widetilde{\beta} = \beta T_{*}, \ \widetilde{\kappa} = \kappa S_{*}, \ \widetilde{\nu} = \nu e^{\widetilde{\kappa}} T_{*}^{\frac{\gamma}{\gamma-1}} / (\varrho_{*}S_{*})$$

$$\widetilde{t} = t/t_{*}, \widetilde{x} = x/x_{*}, \ \widetilde{U} = U/U_{*}, \ \widetilde{P} = P/(\varrho_{*}U_{*}^{2}),$$

$$\widetilde{\varrho} = \varrho/\varrho_{*}, \ \widetilde{W} = W/W_{*}$$
(51)

$$\frac{d}{d\tilde{t}}\widetilde{T} - \frac{1}{\tilde{\beta}}\left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right)\operatorname{div}_{\tilde{x}}\widetilde{U} = 0,$$

$$\frac{d}{d\tilde{t}}\widetilde{U} + \left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right)\nabla_{\tilde{x}}\widetilde{P} = \widetilde{g},$$

$$\frac{d}{d\tilde{t}}\widetilde{Q} + \left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right)\left(-\frac{1}{\widetilde{T}\widetilde{\beta}}\widetilde{Q} + \widetilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}}\exp\left(-\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\widetilde{T}} - 1\right)\right)\right)\right) \operatorname{div}_{\tilde{x}}\widetilde{U} = 0,$$

$$\frac{d}{d\tilde{t}}\left(\widetilde{W} - \widetilde{Q}\right) + \left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right)\left(\widetilde{P} + \frac{1}{\widetilde{\beta}\widetilde{T}}\widetilde{Q} - \widetilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}}\exp\left(\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\widetilde{T}} - 1\right)\right)\right)\right) \operatorname{div}_{\tilde{x}}\widetilde{U} = 0,$$

Let us now introduce the parameter of convection production

$$\xi^2 = \frac{\widetilde{W} - \widetilde{Q}}{\widetilde{Q}} \tag{53}$$

provided that the energy is excessive  $\widetilde{W} - \widetilde{Q} > 0$ . Now in the variables  $\left(\xi, \widetilde{U}, \widetilde{T}, \widetilde{Q}\right)$  the last equation assumes the form

$$\frac{d}{d\tilde{t}}\left(\widetilde{W}-\widetilde{Q}\right) + \left(1+\widetilde{\beta}\left(\widetilde{T}-1\right)\right)\left(\widetilde{P}-\frac{1}{\widetilde{\beta}\widetilde{T}}\widetilde{Q}+\widetilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}}\exp\left(-\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\widetilde{T}}-1\right)\right)\right)\right) \operatorname{div}_{\widetilde{x}}\widetilde{U} = (54)$$

$$= 2\xi\widetilde{Q}\left\{\frac{d}{d\tilde{t}}\xi + \frac{1}{\xi\widetilde{Q}}\left[-\xi^{2}\left(1+\widetilde{\beta}\left(\widetilde{T}-1\right)\right)\left(-\frac{1}{\widetilde{T}\widetilde{\beta}}\widetilde{Q}+\widetilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}}\exp\left(-\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\widetilde{T}}-1\right)\right)\right)\right) + \left(1+\widetilde{\beta}\left(\widetilde{T}-1\right)\right)\left(\widetilde{P}+\frac{1}{\widetilde{\beta}\widetilde{T}}\widetilde{Q}-\widetilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}}\exp\left(-\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\widetilde{T}}-1\right)\right)\right)\operatorname{div}_{\widetilde{x}}\right]\widetilde{U}\right\} = 0$$

Finally, in the dimensionless variables we get

$$\frac{d}{d\tilde{t}}\widetilde{T} - \frac{1}{\tilde{\beta}}\left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right) \operatorname{div}_{\tilde{x}}\widetilde{U} = 0,$$

$$\frac{d}{d\tilde{t}}\widetilde{U} + \left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right) \nabla_{\tilde{x}}\widetilde{P} = \widetilde{g},$$

$$\frac{d}{d\tilde{t}}\widetilde{Q} + \left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right) \left(-\frac{1}{\tilde{T}\tilde{\beta}}\widetilde{Q} + \tilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}} \exp\left(-\tilde{\kappa}\left(\frac{\widetilde{Q}}{\tilde{T}} - 1\right)\right)\right) \operatorname{div}_{\tilde{x}}\widetilde{U} = 0,$$

$$\frac{d}{d\tilde{t}}\xi + \frac{1}{\xi\widetilde{Q}}\left[-\xi^{2}\left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right) \left(-\frac{1}{\tilde{T}\tilde{\beta}}\widetilde{Q} + \tilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}} \exp\left(-\tilde{\kappa}\left(\frac{\widetilde{Q}}{\tilde{T}} - 1\right)\right)\right)\right) + \left(1 + \tilde{\beta}\left(\widetilde{T} - 1\right)\right) \left(\widetilde{P} + \frac{1}{\tilde{\beta}\widetilde{T}}\widetilde{Q} - \tilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}} \exp\left(-\tilde{\kappa}\left(\frac{\widetilde{Q}}{\tilde{T}} - 1\right)\right)\right) \operatorname{div}_{\tilde{x}}\widetilde{U}\right] = 0,$$
(55)

Let us now introduce the viscosity and pump of the internal energy. The viscosity of a liquid, which is known to decrease with increasing temperature, can be expressed using the Frenkel–Andrade formula

$$\eta = C e^{\frac{E_{\text{visc}}}{RT}} \tag{56}$$

where R is the gas constant,  $E_{\text{visc}}$  is the viscosity activation energy. >From the averaged values of the chosen constants C and  $E_{\text{visc}}$  one calculates the viscosity with various temperatures by (56). In the dimensionless variables, the Frenkel–Andrade formula assumes the form

$$\eta/\eta_* = \varepsilon \exp\left(\frac{\widetilde{E_{\text{visc}}}}{R} \left(\frac{1}{\widetilde{T}} - 1\right)\right)$$
(57)

where  $E_{\text{visc}}/(RT) = \tilde{E}_{\text{visc}}/(R\tilde{T})$ ,  $T/T_* = \tilde{T}$ ,  $\varepsilon = \eta_* L_*/U_* \varrho_*$ ,  $\varepsilon = 1/Re_*$ ,  $Re_*$  is the Reynolds number of the perturbed homogeneous medium. In what follows, we shall

only be concerned with the dynamics of liquid,

$$\frac{d}{dt}\widetilde{T} - \frac{1}{\widetilde{\beta}}\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)\operatorname{div}_{\widetilde{x}}\widetilde{U} = 0,$$

$$\frac{d}{dt}\widetilde{U}_{1} - \frac{1}{\widetilde{\varrho}}\partial_{\widetilde{x}_{1}}\left(\frac{1}{\widetilde{\beta}}\frac{\widetilde{Q}}{\widetilde{T}} - \widetilde{g}\widetilde{x}\frac{1}{\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)^{2}}\right) = \\
= \varepsilon\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)\exp\left(\frac{\widetilde{E}_{\operatorname{visc}}}{R}\left(\frac{1}{\widetilde{T}} - 1\right)\right)\Delta\widetilde{U}_{1} + \widetilde{g}, \\
\frac{d}{dt}\widetilde{U}_{j} - \frac{1}{\widetilde{\varrho}}\partial_{\widetilde{x}_{j}}\left(\frac{1}{\widetilde{\beta}}\frac{\widetilde{Q}}{\widetilde{T}} - \widetilde{g}\widetilde{x}\frac{1}{\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)^{2}}\right) = \\
= \varepsilon\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)\exp\left(\frac{\widetilde{E}_{\operatorname{visc}}}{R}\left(\frac{1}{\widetilde{T}} - 1\right)\right)\Delta\widetilde{U}_{j}, \ j = 2, \dots, n, \\
\frac{d}{dt}\widetilde{Q} + \left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)\left(-\frac{1}{\widetilde{T}\widetilde{\beta}}\widetilde{Q} + \widetilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}}\exp\left(-\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\widetilde{T}} - 1\right)\right)\right) \operatorname{div}_{\widetilde{x}}\widetilde{U} = \\
= \varepsilon\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)\exp\left(\frac{\widetilde{E}_{\operatorname{visc}}}{R}\left(\frac{1}{\widetilde{T}} - 1\right)\right)\Delta\widetilde{Q}, \\
\frac{d}{dt}\xi + \left[\frac{\xi}{2\widetilde{\varrho}\widetilde{Q}}\left(\frac{\widetilde{Q}}{\widetilde{T}}\frac{1}{\widetilde{\beta}} - \widetilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}}\exp\left(-\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\widetilde{T}} - 1\right)\right)\right) + \\
+ \frac{1}{2\widetilde{\varrho}\widetilde{Q}\xi}\left(\widetilde{g}\widetilde{x}\frac{1}{\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)^{2}} - \widetilde{\nu}\widetilde{T}^{\frac{2\gamma-1}{\gamma-1}}\exp\left(-\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\widetilde{T}} - 1\right)\right)\right)\right) \operatorname{div}_{\widetilde{x}}\widetilde{U}\right] = \\
= \frac{1}{\widetilde{\ell^{2}}}\sum_{j=1}^{n} \partial_{\widetilde{x}_{j}}\left[\frac{\widetilde{D}}{\widetilde{T}}\partial_{\widetilde{x}_{j}}\left(\frac{\widetilde{Q}}{\left(1 + \widetilde{\beta}\left(\widetilde{T} - 1\right)\right)^{2}} g_{\xi}(\xi) - \varepsilon^{2}\operatorname{div}_{\widetilde{x}} \cdot A\nabla_{\widetilde{x}}\xi\right)\right]$$

 $D_* \varrho_* = D/(T_* U_*), \widetilde{D} = D/D_*$ . In a field of gravity, the surface tension is inhomogenous

$$A = \begin{pmatrix} a(T) & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1 \end{pmatrix}, \quad a > 1.$$
(59)

The dependence of a(T) on T will be refined when specializing to the two-dimensional model. A possible variant of such a dependence is given in [54].

#### 7 Numerical experiment. The one-dimensional model

In contrast to two- or three-dimensional models, the one-dimensional model is incapable of demonstrating the development of a Rayleigh–Bénard instability with nucleation of vortex-type structures. However, with the use of a one-dimensional model it is most simple to trace, in a numerical experiment, the response of a system to perturbations, which are eventually responsible for the onset and development of vortex structures of a convective flow.

Thus, in the one-dimensional case, in the dimensionless variables the model assumes the form

$$\begin{split} & \tilde{\varrho} \frac{d}{d\tilde{t}} \widetilde{T} - \frac{1}{\tilde{\beta}} \partial_{\tilde{x}} \widetilde{U} = 0, \end{split}$$
(60)  
$$& \frac{d}{d\tilde{t}} \widetilde{U} - \frac{1}{\tilde{\varrho}} \partial_{\tilde{x}} \left( \frac{1}{\tilde{Q}} \frac{\widetilde{Q}}{\tilde{T}} - \widetilde{g} \widetilde{x} \frac{1}{\left(1 + \widetilde{\beta}\left(\tilde{T} - 1\right)\right)^{2}} \right) = \\ & = \varepsilon \left( 1 + \widetilde{\beta}\left(\tilde{T} - 1\right) \right) \exp\left(\frac{\widetilde{E}_{\text{visc}}}{R} \left(\frac{1}{\tilde{T}} - 1\right) \right) \partial_{\tilde{x}}^{2} \widetilde{U} + \widetilde{g}, \\ & \frac{d}{d\tilde{t}} \widetilde{Q} - \frac{1}{\tilde{\varrho}} \left( \frac{\widetilde{Q}}{\tilde{T}} \frac{1}{\beta} - \widetilde{\nu} \widetilde{T}^{\frac{2\gamma-1}{\gamma-1}} \exp\left( -\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\tilde{T}} - 1\right) \right) \right) \partial_{\tilde{x}} \widetilde{U} = \\ & = \varepsilon \left( 1 + \widetilde{\beta}\left(\tilde{T} - 1\right) \right) \exp\left(\frac{\widetilde{E}_{\text{visc}}}{R} \left(\frac{1}{\tilde{T}} - 1\right) \right) \partial_{\tilde{x}}^{2} \widetilde{Q} \\ & \frac{d}{d\tilde{t}} \xi + \left[ \frac{\xi}{2\widetilde{\varrho}\widetilde{Q}} \left( \frac{\widetilde{Q}}{\tilde{T}} \frac{1}{\beta} - \widetilde{\nu} \widetilde{T}^{\frac{2\gamma-1}{\gamma-1}} \exp\left( -\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\tilde{T}} - 1\right) \right) \right) \right) + \\ & + \frac{1}{2\widetilde{\varrho}\widetilde{Q}\xi} \left( \widetilde{g} \widetilde{x} \frac{1}{\left(1 + \widetilde{\beta}\left(\tilde{T} - 1\right)\right)^{2}} - \widetilde{\nu} \widetilde{T}^{\frac{2\gamma-1}{\gamma-1}} \exp\left( -\widetilde{\kappa}\left(\frac{\widetilde{Q}}{\tilde{T}} - 1\right) \right) \right) \right) \partial_{\tilde{x}} \widetilde{U} \right] = \\ & = \frac{1}{\tilde{\varrho}^{2}} \left( \partial_{\tilde{x}} \left[ \frac{\widetilde{D}}{\tilde{T}} \partial_{\tilde{x}} \left( \frac{\widetilde{Q}}{\left(1 + \widetilde{\beta}\left(\tilde{T} - 1\right)\right)^{2}} g_{\xi}(\xi) - \varepsilon^{2} \partial_{\tilde{x}}^{2} \xi) \right) \right], \\ & \quad d_{\tilde{t}} = \partial_{\tilde{t}} + \widetilde{U} \partial_{\tilde{x}}, \quad \widetilde{\varrho} = \frac{1}{\left(1 + \widetilde{\beta}\left(\tilde{T} - 1\right)\right)} \\ & \nu_{B} = \frac{\widetilde{g}}{\widetilde{Q}} \left( \frac{\widetilde{X}}{\left(1 + \widetilde{\beta}\left(\tilde{T} - 1\right)\right)} - 1 \right) \end{aligned}$$

where k is the Boltzmann constant,  $\gamma$  is the adiabatic constant, and  $\tilde{g}$  is the acceleration of gravity.

On the interval  $\tilde{x} \in [0, 1]$ , we consider the self-excitation of a (convection)-homogeneous state  $\xi_0^0 = 0.5$ ,  $U_0^0 = 1$ ,  $Q_0^0 = 4$ ,  $T_0^0 = 3$ :

1) either by controlling from the left by the temperature (on the lower surface  $\tilde{x} = 0$ )

$$\widetilde{T}|_{\widetilde{x}=0} = \widetilde{T}_0^0 + V_T t, \ \widetilde{Q}|_{\widetilde{x}=0} = \widetilde{Q}_0^0 \ge 1,$$

$$\widetilde{Q}_0^0 = 4 \ge 1, \quad \widetilde{T}_0^0 = 3 \ge 1, \ , \ V_T = 2;$$
(62)



Figure 6: Numerical solution of the system  $(\xi)$  with  $\xi_0^0 = 0.5, U_0^0 = 1, Q_0^0 = 4, T_0^0 = 3, V = 2$ : (a) the time section t = 0; (b) the time section t = 0.0025; (c) the time section t = 0.005; (d) the time section t = 0.0075.

the initial value  $\xi_0 = 0.5$  is chosen from the lability zone for the potential for

$$\nu_B^0 = \frac{\widetilde{g}}{\widetilde{Q}_0^0} \left( \frac{\widetilde{x}_0}{\left(1 + \widetilde{\beta} \left(\widetilde{T}_0^0 - 1\right)\right)} - 1 \right) < 0$$

2) or by controlling from the left by the heat

$$\widetilde{Q}|_{\widetilde{x}=0} = \widetilde{Q}_0^0 + V_Q t, \quad \widetilde{T}|_{\widetilde{x}=0} = \widetilde{T}_0^0,$$

$$\widetilde{Q}_0^0 = 4 \ge 1, \quad \widetilde{T}_0^0 = 3 \ge 1 \ , \ V_Q = 2$$
(63)

Below, we shall give the time sections t = 0; 0.0025; 0.005; 0.0075; 0.01 for the graphs for the parameter of convection production  $\xi$ , temperature T, heat Q and velocity Ufor the first case (62) of self-excitation of the (convection)-homogeneous state.

Figure 6 shows the development of perturbation, which was initially defined,  $\xi|_{t=0} \equiv \xi_0$ , on the interval  $x \in [0, 1]$ . An increase of the temperature on the lower surface  $\tilde{x} = 0$  (by the condition (62)) results in a convective instability on the upper surface  $\tilde{x} = 1$ , which points to the nonlocality of the perturbation. This, in turn, shows that this problem is not amenable to the classical theory of perturbations.

As already noted above, the thermodynamic analysis is capable of concluding that the upper layers of liquid are more convective unstable than the lower ones, with the proviso that the "kinetic" factors (like the heat conduction and viscosity) may substantially alter the situation. Thus, in a given system there may develop a great number of various scenarios due the differences in the thermodynamic and kinetic contributions on different development stages of the convection process. This is supported by preliminary calculations. No convective instability is observed *ab initio* on the lower surface, because during this time the propensity to buoying (which is necessary for the development of a convective instability) is hindered by the heat conduction. Later, an oscillation develops on the boundary heated region (*viz.*, a convective instability, because the conduction does not secure the leveling of the temperature, and as a corollary, of the density). Hence, here the convective flow is consequent on the development of the upward buoyancy force (the "negative" gravitation force).

In Figs. 7 we show the development of the perturbations of T, U and Q, with the initial data  $T|_{t=0} \equiv T_0, U|_{t=0} \equiv U_0$ , on the interval  $x \in [0, 1]$ . Perturbations on the upper surface  $\tilde{x} = 1$  are hindered by the viscosity.



Figure 7: (a) and (b)-Numerical solution of the system (*T* is the temperature) with  $\xi_0^0 = 0.6, U_0^0 = 0, Q_0^0 =, T_0^0 =, V = 20$ : (a) the time section t = 0.0025, (b) the time section t = 0.01; (c) and (d)-Numerical solution of the system (*U* is the velosity) with  $\xi_0^0 = 0.6, U_0^0 = 0, Q_0^0 =, T_0^0 =, V = 20$ : (c) the time section t = 0.0025, (d) the time section t = 0.01.

To explain the potentiality for the system under consideration to transit in the large from a thermally inhomogenous (but convectively stable) state to a convectively unstable one, we again consider Fig. 5b and draw on it the vertical line corresponding to the initial value of the parameter of convection production  $\xi = \xi_0$ . We see that, as the modulus of the Bénard constant  $|\nu_B|$  decreases with increasing temperature  $\tilde{T}$ , in the first boundary-value condition (62) (respectively,  $\tilde{Q}$  in the second boundary-value condition (63)) the vertical line goes form the stable zone to the lability zone; that is, it crosses the portion of the graph for the free Gibbs energy between inflection points.



Figure 8: Numerical solution of the system ( $S_t$  is the entropy production) with  $\xi_0^0 = 0.6$ ,  $U_0^0 = 0$ ,  $Q_0^0 = T_0^0 =$ , V = 20: (a) the time section t = 0, (b) the time section t = 0.0025, (c) the time section t = 0.005, (d) the time section t = 0.0075.



Figure 9: Sections of the graph of the resulting potential  $\hat{g}_B^{(1)}$ : for  $|\nu_B| = 0.16; 0.11; 0.06; 0.01$ 

The penetration into the lability zone results in a stall from the local equilibrium due to the onset of oscillations of the convective instability (nonlocal perturbation).

It is worth noting that the onset and development of a Rayleigh–Bénard convective instability differs substantially from the laminar-turbulent transition and a transition to the developed turbulence [50].

For a laminar-turbulent transition, the model of [50] gives the following scenario. In the case when the support tangent has a negative slope with the graph of  $\tilde{g}$  and if  $\xi_0^0$  are the initial conditions, then the regime of rapid transitions to turbulence is characteristic of the core of the lability zone; in its developed form this regime has similarities with the process in the "predator-prey" model; that is, an intermittencytype "volatility" is realized [53]. With  $t \to \infty$  the flow is stabilized; that is, changes to the regime in which  $\xi(x,t) \to \xi_{\infty} \left(\frac{x-U_{\infty}t}{\varepsilon}\right)$  tends to the traveling wave  $\xi_{\infty} \left(\frac{x-V_{\infty}t}{\varepsilon}\right)$ , where  $\xi_{\infty}(x)$  is a strictly monotone decreasing (kink-like) function with the boundary values  $\xi|_{x=0} = \xi_{\infty}^{+} > 0$ ,  $\xi|_{x=1} = \xi_{\infty}^{-} < 0$  (an analogue of the solution to the Kolmogorov– Petrovskii–Piskunov (KPP) equation). If the slope between the support tangent and the graph of  $\tilde{g}$  is positive, then self-excitation of turbulence develops by an order faster than in the previous case of a negative slope, the process tending to the one with homogeneous distribution of the turbulization parameter  $\xi(x,t) \to \xi_{\infty}$ . In such a way, the flow arrives at the state of developed turbulence ( $\xi \equiv \text{const}$ ); that is, to the state with excess energy  $\xi_{\infty} > \xi_{0}^{0}$ . This scenario can be illustrated by the description of L. G. Loitsianskii's experimental results [53]. To support this, we give a few quotes from [53] (p. 587).

"A careful examination of the flow in a tube with near-critical Reynolds numbers shows that in the same fixed section of the tube and with the same value of the Reynolds number  $Re = U_{cr}d/\nu$ , the laminar and turbulent regimes may interchange. This phenomenon is now known as intermittency... The cause of the intermittency of flow regimes is that the turbulence... is first formed in discrete regions of the flow like "small clouds" or "spots", which for a tube may fill the transverse section of the pipe "plugs", whose length in the longitudinal direction, which is a function of the Reynolds number of the flow, may be about several tends of the pipe diameter.

The fraction of time during which there exists the turbulent regime in a given section of a tube is the principal quantitative characteristic of intermittency. This dimensionless quantity, which is 0 if the flow is always laminar and is 1 if the flow retains the turbulent form, is called the "intermittency factor"... $\gamma$ . This quantity depends both on the Reynolds number of the flow and on the distance x from the tube inlet... The intermittency factor sharply increases in the region of critical Reynolds numbers (later away from the pipe inlet)." "... forward edges of plugs with supercritical regimes move faster that the backward edges, which causes the "plugs" to extend and fill during their motion more and more space in the tube. At the same time, the forward edge of one "plug" reaches the backward edge of the adjacent "plug". The result of all this is that a continuous turbulent flow is set under supercritical values of Re away from the tube inlet." "At first, the velocity of the "plug" front wall is smaller, but as the Reynolds number increases, it becomes larger than that of the turbulent flow on the tube axis, whereas the velocity of the back wall is much smaller than this velocity. It is also worth pointing out that, in contrast, below the critical value of the Reynolds number, the velocity of the forwards edge of a "plug" is smaller than that of the backward edge; this results in a decrease of the lengths of the resulting "plugs" and their disappearance in the laminar flow." This qualitative description of the experimental results of [53] perfectly matches the results of [50]. In the first case, the turbulization front moves along the flow with some velocity, which in fact is the onset rate of the fraction of the "turbulent" liquid. The same phenomenon takes place on the back wall, and hence in the laboratory coordinate system the back wall moves upstream, but at the same time it is stalled by the flow. Here, the phase transition changes from the laminar to the turbulent flow. This situation reverses for subcritical regimes: nuclei of "turbulent" liquid "dissolve" in the nonturbulent one; the phase transition being directed from the

regime laminar regime (relaminarization).

For a Rayleigh–Bénard convective instability the situation is different, because two lability zones may exist; that is, two counter-current process of convection may develop—they start from the lower ( $\tilde{x} = 0$ ) and the upper surface ( $\tilde{x} = 1$ ) with unperturbed central region. On the lower surface, where the gravitation is "negative" and small, the heat conduction is significant on the initial stage of the perturbation development. Convective perturbations first develop on the upper boundary, when the heating of the entire liquid layer (of sufficient height) becomes substantial and when the heat conduction is incapable of removing the gradient of the temperature, and, respectively, the densities over the layer height. Such a behavior can be revealed within the one-dimensional model. In the multi-dimensional model (two-dimensional or three-dimensional ones), the development of perturbations in the vertical direction from the upper and lower surfaces with their mutual horizontal displacement must result in the appearance of rotational motions and eventually in the formation of Bénard cells. The appearance of such motions in the upper layer of liquid may result in the formation of a thermal inhomogeneity of the upper surface, and in turn, in an alternating inhomogeneity of the surface tension, since it depends on the temperature. As a result, a Bénard–Marangoni instability may develop, which strengthens the effect of the original Rayleigh–Bénard instability.

We hope to treat this phenomenon in a forthcoming paper.

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Received 01.05.2017, Accepted 22.05.2017